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REPORT AMCPEO CDE-88004

CHEMICAL STOCKPILE DISPOSAL PROGRAM

CENTIFY

A COMPUTER PROGRAM FOR THE ANALYSIS OF LABORATORY DATA

1 OCTOBER 1988

PROGRAM MANAGER
FOR CHEMICAL DEMILITARIZATION

EDGEWOOD PROVING GROUND, MARYLAND 21010-5401

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An IBM-PC based computer program for the analysis of laboratory data for the Program Manager for Chemical Demilitarization. The program performs a weighted least squares regression of laboratory certification data and provides both text and graphical reports. Data analysis includes linear regression of data, outlier testing, confidence bounds and operating characteristic curves.

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CERTIFY

Version 1.01

An IBM-PC Based Computer Program for the Analysis of Laboratory Data for the Program Manager for Chemical Demilitarization

Prepared by:

Systems Engineering Office
PM Cml Demil
APG, MD 21010-5401

October 1988

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1. INTRODUCTION

CERTIFY is a computer program which can be used to analyze toxic agent air monitoring data. Its specific purpose is to certify laboratory methods as meeting precision and accuracy requirements as established by the Department of Health and Human Services (DHHS), the Environmental Protection Agency (EPA) and other regulatory organizations.

CERTIFY requires the following to run:

- IBM PC, XT, AT or Compatible.
- One 1.2 MB Floppy Drive or Hard Drive (hard drive recommended).
- 256K Ram Memory.
- Color Graphics Adapter or Enhanced Graphics Adapter
- IBM Graphics Printer or Compatible.

CERTIFY can process data files containing up to 3500 data points. Input data may be in any units but output generated by CERTIFY is in terms of 1 hazard level or 1 Z. The use of Z and hazard level are treated as synonymous.

2. GETTING STARTED

2.1 Installing CERTIFY on your hard drive.

-- Load DOS on your computer.

- Place the CERTIFY disk in drive A.
  (If drive A is a 360kb drive place disk 1 in drive A)

- From the DOS Directory on drive C:

  Type - A:INSTALH §RETURN¶

This procedure will place the program files in a subdirectory named CERTIFY.

2.2 Prior to Running

Prior to running CERTIFY the graphics drivers required for screen dumps and extended graphics characters for your screen and to your printer must be loaded. For IBM PC's these drivers are called GRAFTABL.COM and GRAPHICS.COM. Both must be loaded prior to running CERTIFY. To load the extended characters type GRAFTABL and §RETURN¶. To load the screen graphics type GRAPHICS and §RETURN¶. Some printers such as the Calcomp Colormaster require separate drivers to allow screen dumps. If there are any questions regarding your printer, refer to your printers user's manual.

2.3 Running CERTIFY

2.3.1 From your Hard Drive

Type CD CERTIFY §RETURN¶
Type CERTIFY §RETURN¶

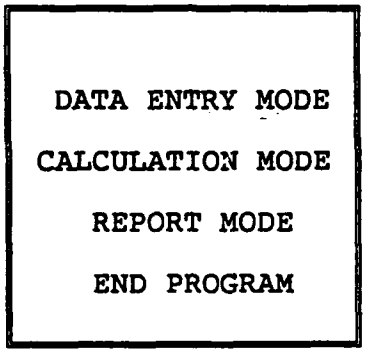
2.3.2 From a 1.2 Mb Floppy Drive. Place the 1.2 Mb Floppy with CERTIFY on it into the high density drive.

Type CERTIFY §RETURN¶

Creation of files on the 1.2 Mb floppy drive may cause the capacity limit of the diskette to be exceeded during execution. For this reason, insure that *.CER files on the disk are frequently transferred to another high density diskette and deleted from the CERTIFY diskette.

3. INPUT

Most input to CERTIFY is menu driven. The main menu is shown in Figure 1.



USE UP AND DOWN ARROWS TO CHOOSE

PRESS ENTER TO MAKE SELECTION

Figure 1. Main Menu

From the Main Menu, use the up or down arrow keys to highlight DATA ENTRY MODE and press enter. At the next menu, (figure 2) highlight CREATE A DATA FILE and press enter.

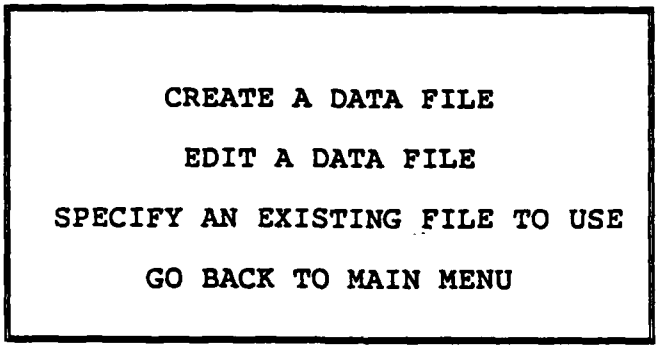


Figure 2. Data Mode Menu

You will be asked to input a data file name to create. Type a descriptive file name of not more than 8 characters. Do not include any extensions. CERTIFY will give the data file the extension .CER automatically. Next, you will be prompted for the following five items:

Example

AT THIS TIME ENTER LINES OF DESCRIPTIVE TEXT FOR THIS DATA FILE
DO NOT EXCEED ONE LINE OF TEXT FOR EACH ENTRY

AGENT: ? VX
ENVIRONMENT: ? STACK
METHOD NAME: ? ACAMS
LABORATORY: ? JACADS
DATES OF ANALYSIS: ? 1-5 FEB 70 6-9 MAR 70

These are required descriptive text only and should not exceed one line.

Next, up to 20 lines of descriptive text may be entered. Again, do not exceed one line each for these entries. This descriptive text can include any items which lend to the understanding of the conditions of the test or other information pertinent to the data set.

Next, the program prompts for the hazard level concentration (Z) and the units. This should be in the same units as the data set. Following input of the hazard level, the program prompts for the number of target concentrations.

This is the number of different target concentrations in the data set and may not exceed 10. Following this entry the actual target concentrations must be entered. Again, the units of these concentrations should be compatible within the data and the values must match exactly with those in the data set. Data need not be input sequentially by group. Grouping by target concentration will be done by CERTIFY.

Example

This is your Data Set

X	Y
.1	.11
.20	.22
.1	.12
.501	.50
.1	.095
.1	.10
.20	.21
.20	.19
.20	.23
.1	.10
.501	.48
.501	.47
.501	.55

Then your Input should be

# of Targets = 3

#1 = .1
#2 = .20
#3 = .501

This completes the header information for the data file.

The next screen is the initial data entry screen and all items must be entered. This screen looks like that shown in Figure 3.

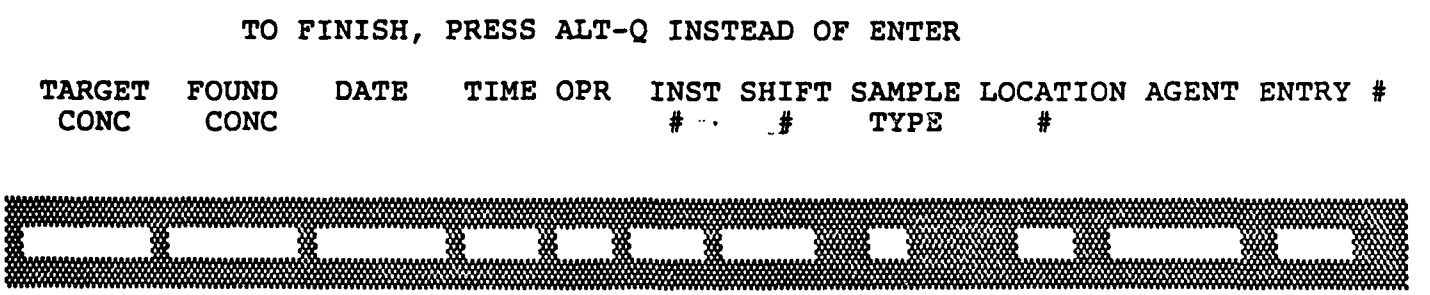


Figure 3. Initial Entry Screen

Prompts will be given to enter each data element.

Once all the elements have been completed press enter to move to the next data entry record. Any element of a data line may be edited until the enter key is pressed. Figure 4 shows the screen prior to ENTER being pressed. Note the entry number has not incremented.

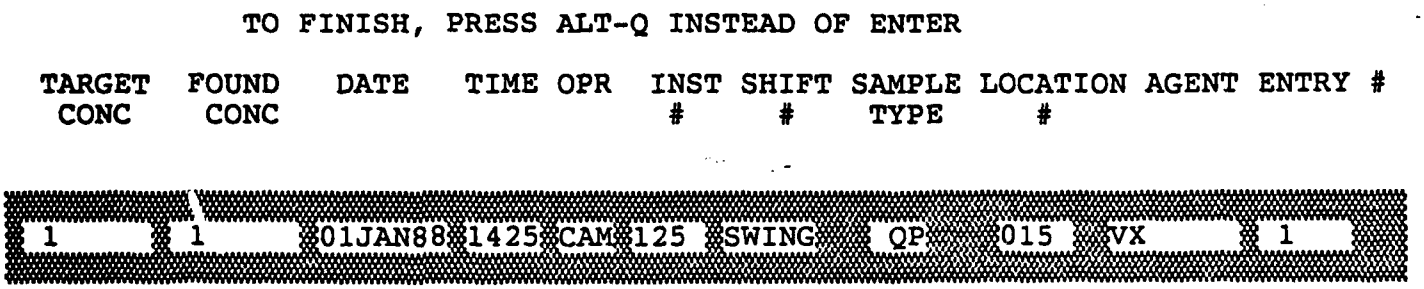


Figure 4

Following the initial entry screen, only the target (x) values and found concentration (y) values are required input. All other elements will retain the value of the last change. The x value must be entered then the y value entered. Again, any element can be changed at this point by pressing the appropriate function key (f key) displayed at the bottom of the screen. Once the data line is correct, press enter.

Mistakes made during the creation of a data file can be edited using the editor described in section 3.2. Once all the data records have been entered, press ALT-Q. This will store the file. If no mistakes were made during input, calculations can be made directly at this point as the current file is the file you just created. The current file will be discussed in section 3.3.

3.2 Editing *.CER files.

The second entry from the data mode menu (figure 2) is edit an existing data file. When this option is selected the first thing that must be done is to select an existing file to be edited. A screen similar to that shown in Figure 5 prompts the user for a file name. It should be noted that only *.CER data files are allowed. The extension .CER is not required to select a file.

```
BELOW ARE THE AVAILABLE DATA FILES.  ONLY X.CER FILES CAN BE USED

C:\USERMENU\CERTIFY
BZDATA  .CER      ACAMS1A .CER      MBENCH2 .CER      TEST    .CER

 23490560 Bytes free


TYPE FILENAME (WITHOUT .CER) OR NONE?
```

Figure 5

After a file is selected the user is prompted for any changes in header information. Figure 6, as an example, shows the screen which would allow changing the dates of the data set. The previous items would have already been either changed or left alone. Following this screen, the hazard level concentration and the target concentrations of the data set can be modified in a similar fashion.

FILE: MBENCH2.CER

AGENT: GB

ENVIRONMENT: PERIMETER

METHOD: DAAMS

LABORATORY: CAMDS/EAI

DATES: 12-15 JAN 88

PRESS C TO CHANGE OR ANY OTHER KEY

Figure 6

Next, a screen such as that shown in Figure 7 presents the last record of the selected data file. ALT D and ALT U can be used to move up or down through the data file. The function keys can be used to alter individual fields.

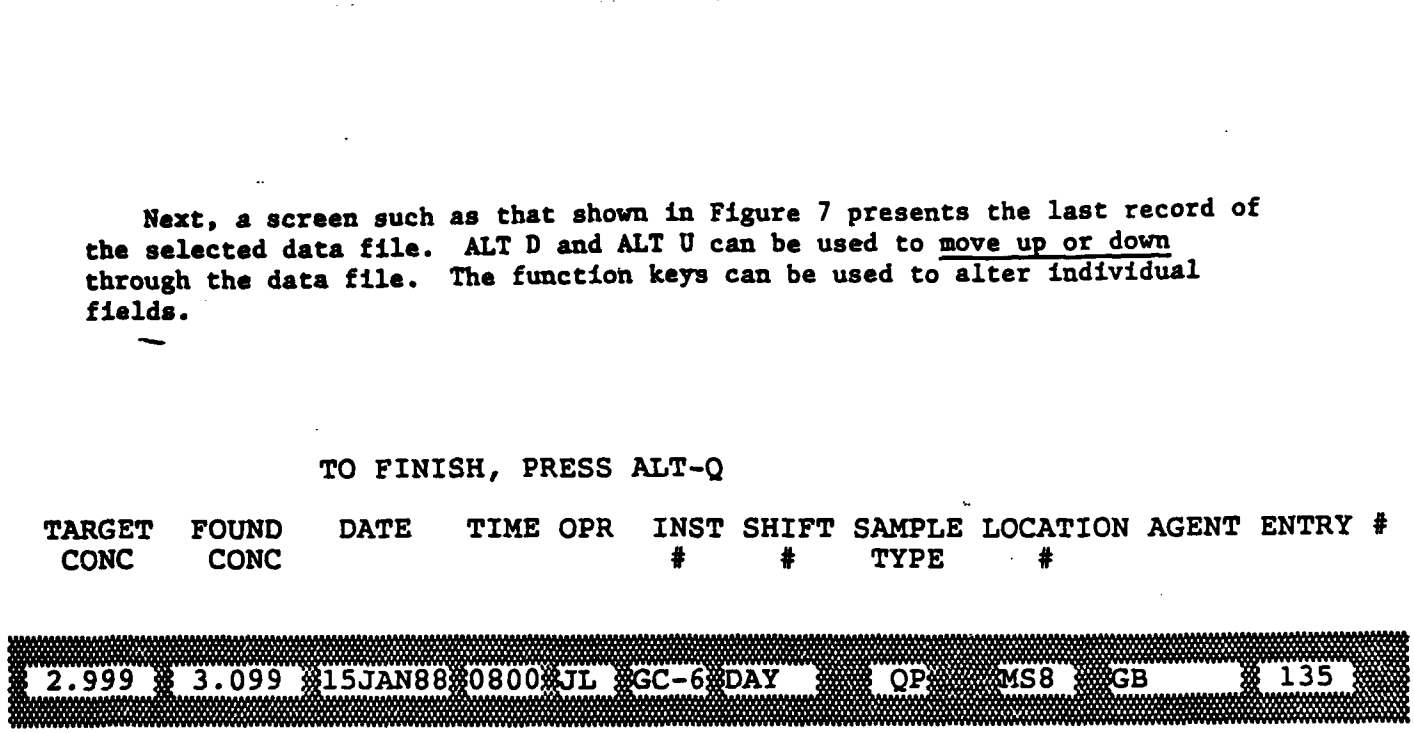


Figure 7

To delete a record, move to that record using ALT-D or ALT-U. Next press ALT-E and then enter. A screen similar to that shown in Figure 8 will show that the record will not be included in calculations. The record itself will remain in the data file. There is no current ability to pack the data. A999 will appear in the target concentration field. This indicates data not to be included.

TO FINISH, PRESS ALT-Q

TARGET CONC	FOUND CONC	DATE	TIME	OPR	INST #	SHIFT #	SAMPLE TYPE	LOCATION #	AGENT	ENTRY #
999	3.044	15JAN88	0800	JL	GC-6	DAY	QP	MS8	GB	134

THIS RECORD NOT TO BE INCLUDED IN CALCULATIONS

USE FUNCTION KEYS TO CHANGE VALUES

ALT-U UP A RECORD ALT-D DOWN A RECORD ALT-E ERASE A RECORD
ALT-A ADD RECORDS

1TARGE 2FOUND 3DATE 4TIME 5OPR 6INST 7SHIFT 8SAMPLE 9LOCATI 10AGENT

Figure 8

To add records press ALT-A. A screen similar to that shown in Figure 9 appears. To begin adding records press enter. X, Y, pairs are entered similar to the process used in creating a data file. To stop adding records press ALT-S when the screen is similar to that shown in Figure 10

TO FINISH, PRESS ALT-Q

TARGET CONC	FOUND CONC	DATE	TIME	OPR	INST #	SHIFT #	SAMPLE TYPE	LOCATION #	AGENT	ENTRY #
2.999	3.099	15JAN88	0800	JL	GC-6	DAY	QP	MS8	GB	135

PRESS ENTER TO START ADDING

USE FUNCTION KEYS TO CHANGE VALUES

PRESS ALT-S TO STOP ADDING

1TARGE 2FOUND 3DATE 4TIME 5OPR 6INST 7SHIFT 8SAMPLE 9LOCATI 10AGENT

Figure 9

TO FINISH, PRESS ALT-Q

TARGET CONC	FOUND CONC	DATE	TIME	OPR	INST #	SHIFT #	SAMPLE TYPE	LOCATION #	AGENT	ENTRY #
1	2	15JAN88	0800	JL	GC-6	DAY	QP	MS8	GB	136

PRESS ENTER TO CONTINUE ADDING

USE FUNCTION KEYS TO CHANGE VALUES

PRESS ALT-S TO STOP ADDING

1TARGE 2FOUND 3DATE 4TIME 5OPR 6INST 7SHIFT 8SAMPLE 9LOCATI 10AGENT

Figure 10

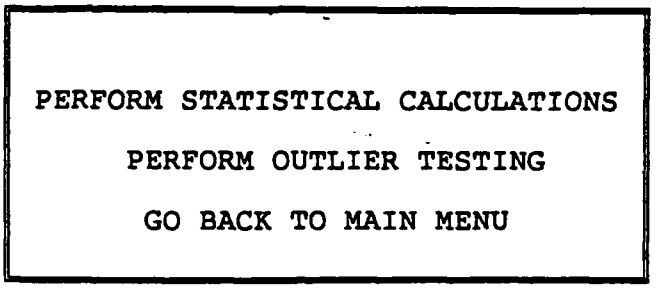
Exiting the editor is the same as exiting the file creation routine, press ALT-Q. The user will be given the option of returning to the editor (by typing R) or going back to the main menu (by pressing any other key). Upon exiting the editor mode, a backup copy of the *.CER file is made. This backup has the same name but the extension is changed to *.BAK.

3.3 Selecting a Data file for calculations.

Calculations are performed based on the current file known to the program. The current file to be used in calculations is automatically set if the create or edit file modes are used. The current file being the one just created or edited. To use an existing file select the 3rd option from the Data Mode Menu (Figure 2). A screen similar to the one shown in Figure 5 will appear allowing the user to select a file to use. Once a file is selected using this mode it becomes the current file.

4. Calculations

Calculations are performed from the calculation mode menu shown in Figure 11.



USE UP AND DOWN ARROWS TO CHOOSE

PRESS ENTER TO MAKE SELECTION

Figure 11

4.1. Statistical Calculations.

Once a current file has been selected, from the main menu (Figure 1), select calculations mode. Next, select the PERFORM STATISTICAL CALCULATIONS from the calculation mode menu (Figure 11). Calculations may take from 1 minute to over 10 min depending on the size and nature of the data set. Graphical output screens allow the user to see the data as it is generated and the program will prompt the user to press any key to continue after presenting each screen. Once calculations are completed the program returns the user to the main menu.

An example of the screen output can be found in the sample report at Appendix A.

The other calculational choice is to perform outlier testing. When outlier testing is performed, outliers are determined from the current file and a new current file is produced with the extension .OLT. An outlier report only can be produced using the report mode which is described in Section 5 or statistical calculations can be performed using the 1st option on the calculation mode menu. Statistical calculations with outliers included should always be conducted and results compared to the results without outliers.

NOTE: The outlier test does not alter the original data file. The only way to make a data file without outliers the current file is to perform the outlier test calculations. Outliers are represented on graphical output as larger open circles.

4.3 Methodology.

Methodology for the weighted regression and confidence bound calculations can be found in Appendix B. Calculation of OC curves can be found in Appendix C and methods of outlier testing can be found in Appendix D.

5. Report Generation

Reports can only be generated after running the calculation mode routine(s). Once calculations are complete, select report mode from the main menu shown in Figure 12.

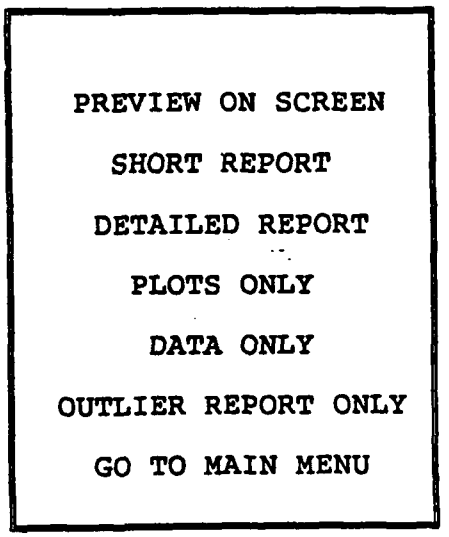


Figure 12

5.1 Preview on Screen

Preview on screen is an onscreen preview of the output. Use this option to look at the results of calculations prior to sending it to the printer.

5.2 Short Report.

The short report provides a printout of the vital statistics from calculations. It includes two header pages, the operating characteristics data for alarm conditions, statistical parameters (to include the results of outlier testing if conducted, and tabulated confidence bounds. The short report provides the necessary information for brief evaluation without graphical display or tabulated data.

5.3 Detailed Report

The detailed report selection from the report menu adds all of the plots and a tabulation of the data set to the short report. Appendix A is an example of a detailed report.

5.4 Plots Only.

This selection produces only the plots generated during calculations. From the report mode menu, selection plots only gives the plots only menu (Figure 13). Any of 5 separate plots may be plotted or all plots may be selected for output. An example of the plots can be found in the detailed report example of Appendix A.

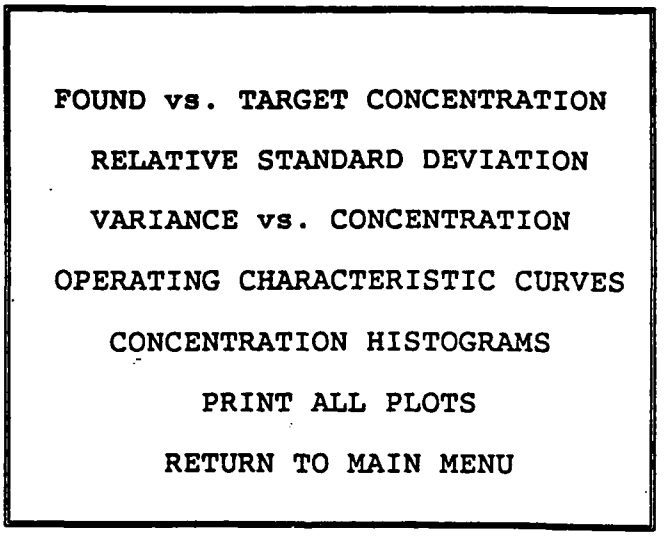


Figure 13

5.5 Data Only.

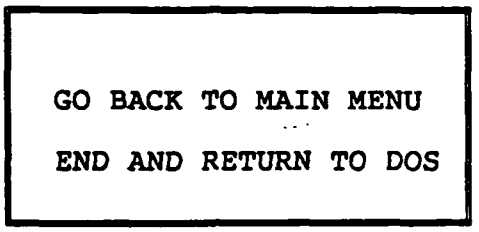
This report menu selection gives a printout of the data. An example can be found following the plots in the detailed report example at Appendix A.

5.6 Outlier Report Only.

Once an outlier test has been conducted and the OLT file is current file and outlier report can be produced. This is only report which can be produced without running statistical calculations from the calculations mode menu. The outlier report (if conducted) is also included in the short and long reports.

6. Ending the Program

CERTIFY should be exited through the main menu only. The end program menu allows the user to return to the main menu or end and return to DOS (Figure 14). Selecting end and return to DOS clears temporary working files from the system and ensures that future calculations are not performed on erroneous temporary files.



USE UP AND DOWN ARROWS TO CHOOSE

PRESS ENTER TO MAKE SELECTION

Figure 14

7. Problems/Questions

Should you encounter problems or simply have questions regarding CERTIFY, contact:

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REPORT SUMMARY PAGE

VERSION 1.01

AGENT: GB

ENVIRONMENT: PERIMETER

METHOD NAME: DAAMS

LABORATORY: CAMDS/EAI

DATES OF ANALYSIS: 12-15 JAN 88

SAMPLE SIZE: 124

TARGET VERSUS FOUND CONCENTRATION SUMARY

FOUND ACTION LIMIT: .8881824

TARGET ACTION LIMIT: .7708484

LIMIT OF QUANTIFICATION: 6.152139E-02

DECISION LIMIT: 2.997687E-02

OVERALL RECOVERY: 101.7282

UNCERTAINTY (with 95% confidence) IN FOUND MASS: ± 12.31415 %

UNCERTAINTY (with 95% confidence) IN AIR SAMPLE: ± 11.4597 %

TARGET LEVELS

1 HAZARD LEVEL (Z) = 1 ng

TARGET LEVEL # 1 = 0 (Z)
TARGET LEVEL # 2 = .1467 (Z)
TARGET LEVEL # 3 = .2935 (Z)
TARGET LEVEL # 4 = .4403 (Z)
TARGET LEVEL # 5 = .7339 (Z)
TARGET LEVEL # 6 = 1 (Z)
TARGET LEVEL # 7 = 2.9999 (Z)

DESCRIPTIVE TEXT FROM DATA FILE MBENCH2.OLT

EAI Corporation conducted this four-day P&A test at CAMDS from 12 to 15 January 1988. The manual DAAMS procedure in Volume 2 of the Analytical Methods Development Report, J.E. Smith, Jr. and W.K. Fowler (Southern Research Institute) was followed. The sampling tubes (Chromosorb 106, 6 mm ID) were manufactured by Combustion Engineering. The DAAMS tubes were aspirated at perimeter station 8 at a flow rate of 500 mL/min for 12 hours. Hewlett-Packard Model 5890 GC's, located in the Site Analysis Facility, were used for analysis (#6 & #7).

EAI Test Officer was Dr. Barry Knier; EAI Analysts were Mr. Jeff Lippert and Ms. Judy Price. CAMDS Test Coordinator was Mr. Bill James; expert technical assistance was also provided by Messrs. Lanny Davis, Tom Marshall, and John McPhie of the CAMDS Monitoring Branch.

****
****
****
****
****
****

PROBABILITY OF ALARM

CONCENTRATION (Z)

INSTRUMENT SETTING	0.2000	0.4000	0.6000	0.8000	1.0000	1.2000	1.4000
0.2	0.5688	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.4	0.0000	0.5881	1.0000	1.0000	1.0000	1.0000	1.0000
0.6	0.0000	0.0000	0.5966	0.9999	1.0000	1.0000	1.0000
0.8	0.0000	0.0000	0.0000	0.6012	0.9994	1.0000	1.0000
1.0	0.0000	0.0000	0.0000	0.0004	0.6040	0.9977	1.0000
1.2	0.0000	0.0000	0.0000	0.0000	0.0030	0.6059	0.9940

ALARM SETTING FOR 95% CONFIDENCE LEVEL = 0.9090
ALARM SETTING FOR 97.5% CONFIDENCE LEVEL = 0.8879
ALARM SETTING FOR 99% CONFIDENCE LEVEL = 0.8632

PROBABILITY OF FALSE ALARM AT CONCENTRATION (Z)

INSTRUMENT SETTING	0.1000	0.3000	0.5000	0.7000	0.9000	1.1000
0.05	0.0023	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.4511	0.0000	0.0000	0.0000	0.0000	0.0000
0.15	0.9952	0.0000	0.0000	0.0000	0.0000	0.0000
0.20	1.0000	0.0001	0.0000	0.0000	0.0000	0.0000
0.25	1.0000	0.0221	0.0000	0.0000	0.0000	0.0000
0.30	1.0000	0.4194	0.0000	0.0000	0.0000	0.0000
0.35	1.0000	0.9466	0.0000	0.0000	0.0000	0.0000
0.40	1.0000	0.9996	0.0023	0.0000	0.0000	0.0000
0.45	1.0000	1.0000	0.0608	0.0000	0.0000	0.0000
0.50	1.0000	1.0000	0.4069	0.0000	0.0000	0.0000
0.55	1.0000	1.0000	0.8604	0.0006	0.0000	0.0000
0.60	1.0000	1.0000	0.9913	0.0114	0.0000	0.0000
0.65	1.0000	1.0000	0.9999	0.1016	0.0000	0.0000
0.70	1.0000	1.0000	1.0000	0.4008	0.0002	0.0000
0.75	1.0000	1.0000	1.0000	0.7801	0.0032	0.0000
0.80	1.0000	1.0000	1.0000	0.9630	0.0277	0.0000
0.85	1.0000	1.0000	1.0000	0.9973	0.1373	0.0001
0.90	1.0000	1.0000	1.0000	0.9999	0.3972	0.0013
0.95	1.0000	1.0000	1.0000	1.0000	0.7169	0.0094

PROBABILITY OF FALSE ALARM
AT ALARM SETTING OF 0.8879 AND TC OF 0.5 Z = 0.000

TARGET CONCENTRATION AT WHICH PROBABILITY OF FALSE ALARM WITH ALARM SETTING OF 0.8879 IS LESS THAN 5 PERCENT (%) = 0.785

STATISTICAL PARAMETERS PAGE

REGRESSION EQUATION

Y INTERCEPT = 5.601049E-04

SLOPE = 1.016722

CORRELATION COEFFICIENT = .9979814

STUDENTS T STATISTIC = 1.9794

PERCENT OF DATA POINTS INSIDE OF CONFIDENCE LIMITS = 99.19355 %

PERCENT OF DATA POINTS INSIDE AT THE HAZARD LEVEL 96 %

ESTIMATE OF CENTRAL MEAN AT HAZARD LEVEL = 101.7282 %

ESTIMATE OF CENTRAL RANGE AT HAZARD LEVEL = 24.6283 %

ESTIMATE OF STANDARD DEVIATION AT HAZARD LEVEL = 3.542586 %

ESTIMATE OF RECOVERY UWL = 105.5731

ESTIMATE OF RECOVERY LWL = 97.88332

ESTIMATE OF RECOVERY UCL = 107.4955

ESTIMATE OF RECOVERY LCL = 95.96088

ESTIMATE OF RANGE UWL = 18.73393

ESTIMATE OF RANGE UCL = 28.10089

RESULTS OF OUTLIER TEST

NUMBER OF OUTLIERS DETECTED = 6
PERMISSIBLE NUMBER OF OUTLIERS = 30
PERCENTAGE OF PERMISSIBLE = 20

SUMMARY OF FOUND OUTLIERS

TARGET CONC	FOUND CONC	KURTOSIS	SKEWNESS	ENTRY #
0.0000	0.0174	3.994	1.633	103
0.0000	0.0165	4.794	1.812	53
0.0000	0.0100	3.550	1.627	85
0.0000	0.0100	4.835	1.968	86
0.0000	0.0091	7.143	2.429	102

TOO FEW DATA POINTS TO CONTINUE TEST FOR ABOVE TARGET
DATA IS PROBABLY NOT NORMAL
KURTOSIS IS 7.143457 AND SKEWNESS IS 2.42901

0.1467	0.0834	8.250	-2.106	4

NO OUTLIERS FOUND FOR TARGET CONCENTRATION 0.2935
KURTOSIS IS 1.990175 AND SKEWNESS IS -.1114795

NO OUTLIERS FOUND FOR TARGET CONCENTRATION 0.4403
KURTOSIS IS 3.942086 AND SKEWNESS IS -1.330055

NO OUTLIERS FOUND FOR TARGET CONCENTRATION 0.7339
KURTOSIS IS 2.208973 AND SKEWNESS IS .1480014

SUMMARY OF FOUND OUTLIERS (CONT.)

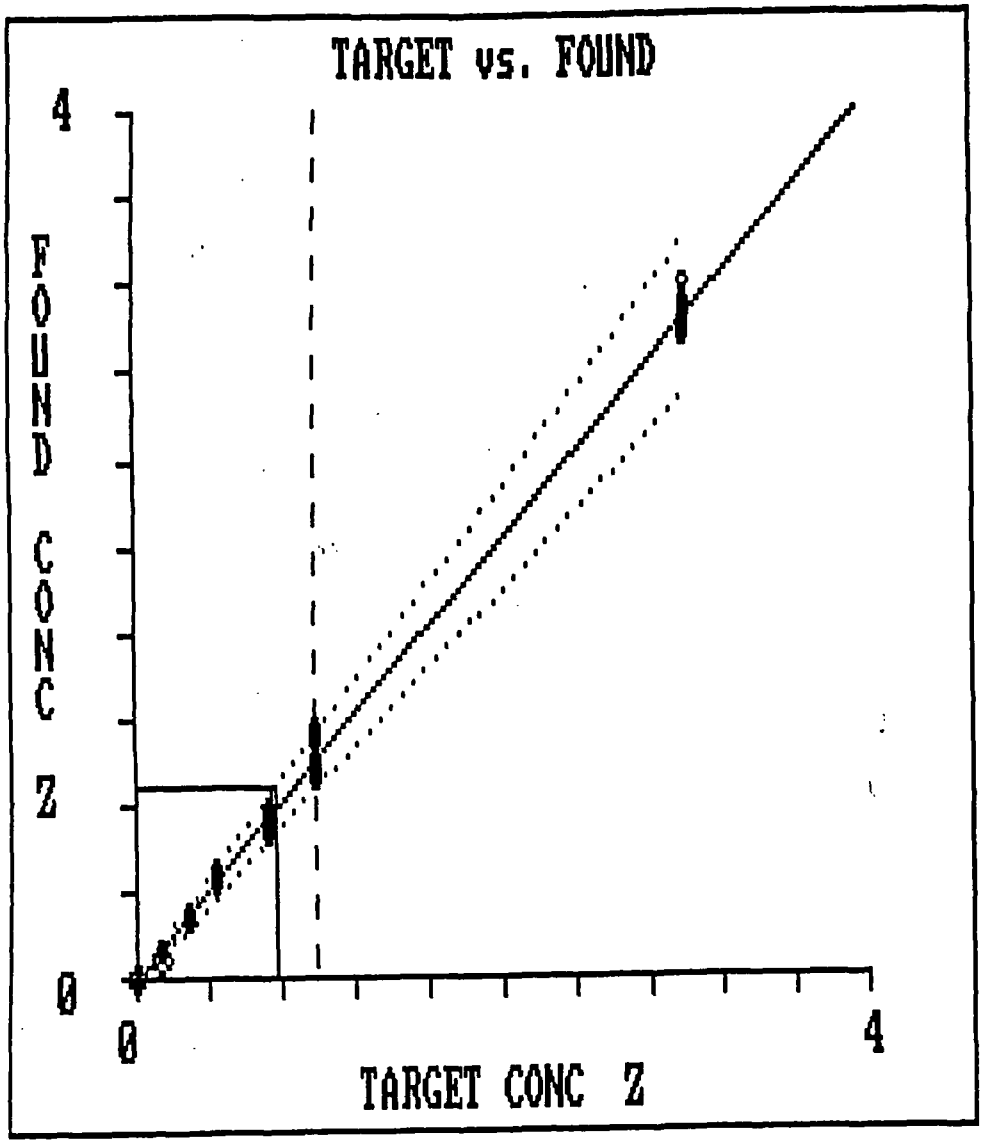
TARGET CONC	FOUND CONC	KURTOSIS	SKEWNESS	ENTRY #

NO OUTLIERS FOUND FOR TARGET CONCENTRATION 1.0000
KURTOSIS IS 2.981791 AND SKEWNESS IS .6531814

NO OUTLIERS FOUND FOR TARGET CONCENTRATION 2.9999
KURTOSIS IS 2.976299 AND SKEWNESS IS .6636055

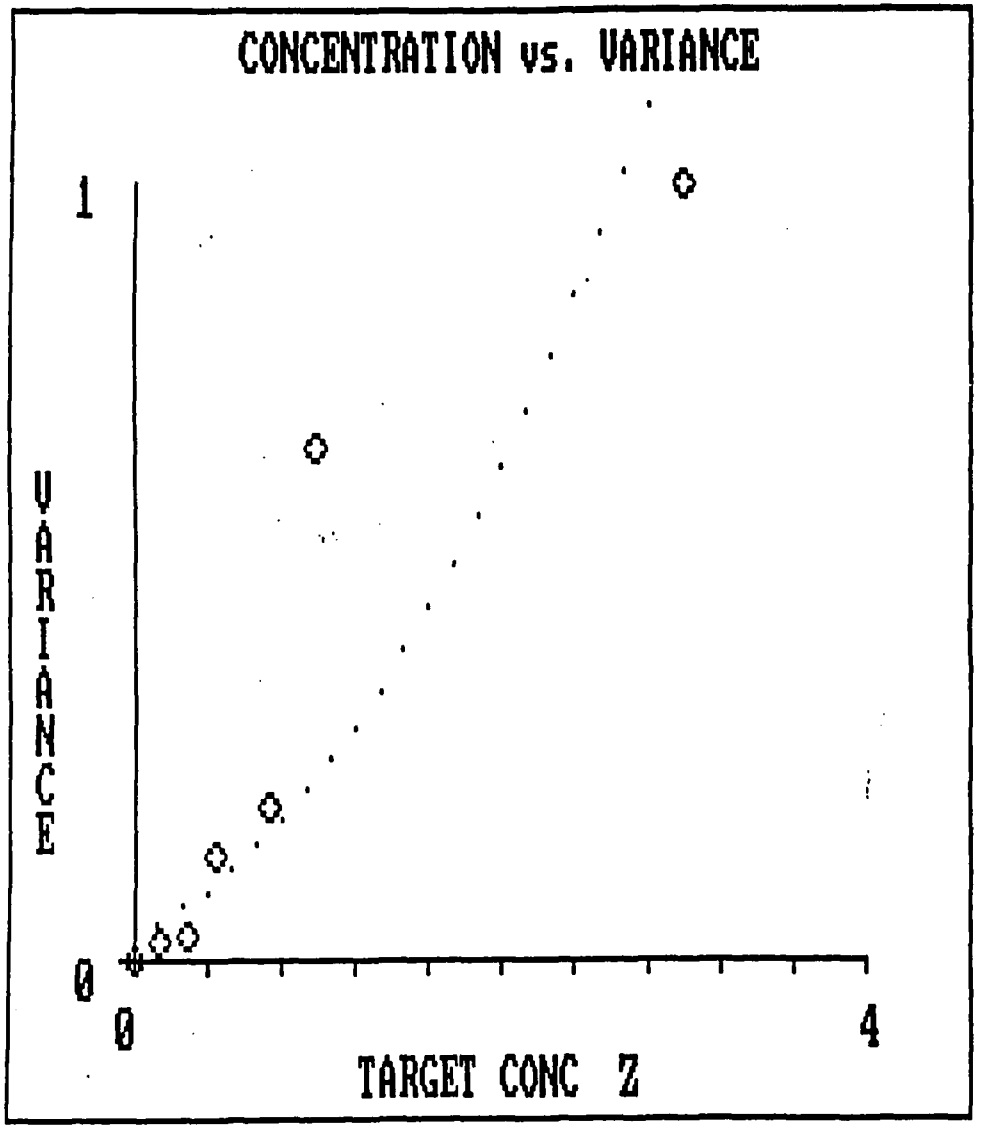
TABULATED CONFIDENCE BOUNDS

TARGET CONCENTRATION (Z)	FOUND CONCENTRATION (Z)	UPPER CONFIDENCE LIMIT	LOWER CONFIDENCE LIMIT
0.0000	0.0006	0.0770	-.0759
0.1000	0.1022	0.1793	0.0252
0.2000	0.2039	0.2828	0.1250
0.3000	0.3056	0.3875	0.2236
0.4000	0.4072	0.4933	0.3212
0.5000	0.5089	0.6000	0.4179
0.6000	0.6106	0.7074	0.5138
0.7000	0.7123	0.8155	0.6090
0.8000	0.8139	0.9241	0.7038
0.9000	0.9156	1.0331	0.7981
1.0000	1.0173	1.1426	0.8920
1.1000	1.1190	1.2523	0.9857
1.2000	1.2206	1.3622	1.0790
1.3000	1.3223	1.4724	1.1722
1.4000	1.4240	1.5827	1.2653
1.5000	1.5256	1.6932	1.3581
1.6000	1.6273	1.8038	1.4509
1.7000	1.7290	1.9145	1.5435
1.8000	1.8307	2.0252	1.6361
1.9000	1.9323	2.1361	1.7285
2.0000	2.0340	2.2471	1.8209
2.1000	2.1357	2.3581	1.9133
2.2000	2.2373	2.4691	2.0056
2.3000	2.3390	2.5802	2.0978
2.4000	2.4407	2.6914	2.1900
2.5000	2.5424	2.8025	2.2822
2.6000	2.6440	2.9138	2.3743
2.7000	2.7457	3.0250	2.4664
2.8000	2.8474	3.1363	2.5585
2.9000	2.9491	3.2476	2.6506
3.0000	3.0507	3.3589	2.7426
3.1000	3.1524	3.4702	2.8346
3.2000	3.2541	3.5816	2.9266
3.3000	3.3557	3.6929	3.0186
3.4000	3.4574	3.8043	3.1105
3.5000	3.5591	3.9157	3.2025
3.6000	3.6608	4.0271	3.2944
3.7000	3.7624	4.1385	3.3863
3.8000	3.8641	4.2500	3.4782
3.9000	3.9658	4.3614	3.5701
4.0000	4.0674	4.4729	3.6620
4.1000	4.1691	4.5843	3.7539
4.2000	4.2708	4.6958	3.8458
4.3000	4.3725	4.8073	3.9376
4.4000	4.4741	4.9188	4.0295
4.5000	4.5758	5.0303	4.1214



AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88

% BIAS (±)	=	11.4597
FAL	=	.8881824
TAL	=	.7708484
LOQ	=	.0615213
DECIS	=	.0299768
% RECOVERY	=	101.7282
DATA POINTS	=	124
SLOPE	=	1.016722
INTERCEPT	=	.0005601
% BIFM (±)	=	12.31415
Z	=	1



MAX VARIANCE= .0053615

VARIANCE 1 = .0007148

VARIANCE 2 = .0237319

VARIANCE 3 = .0266495

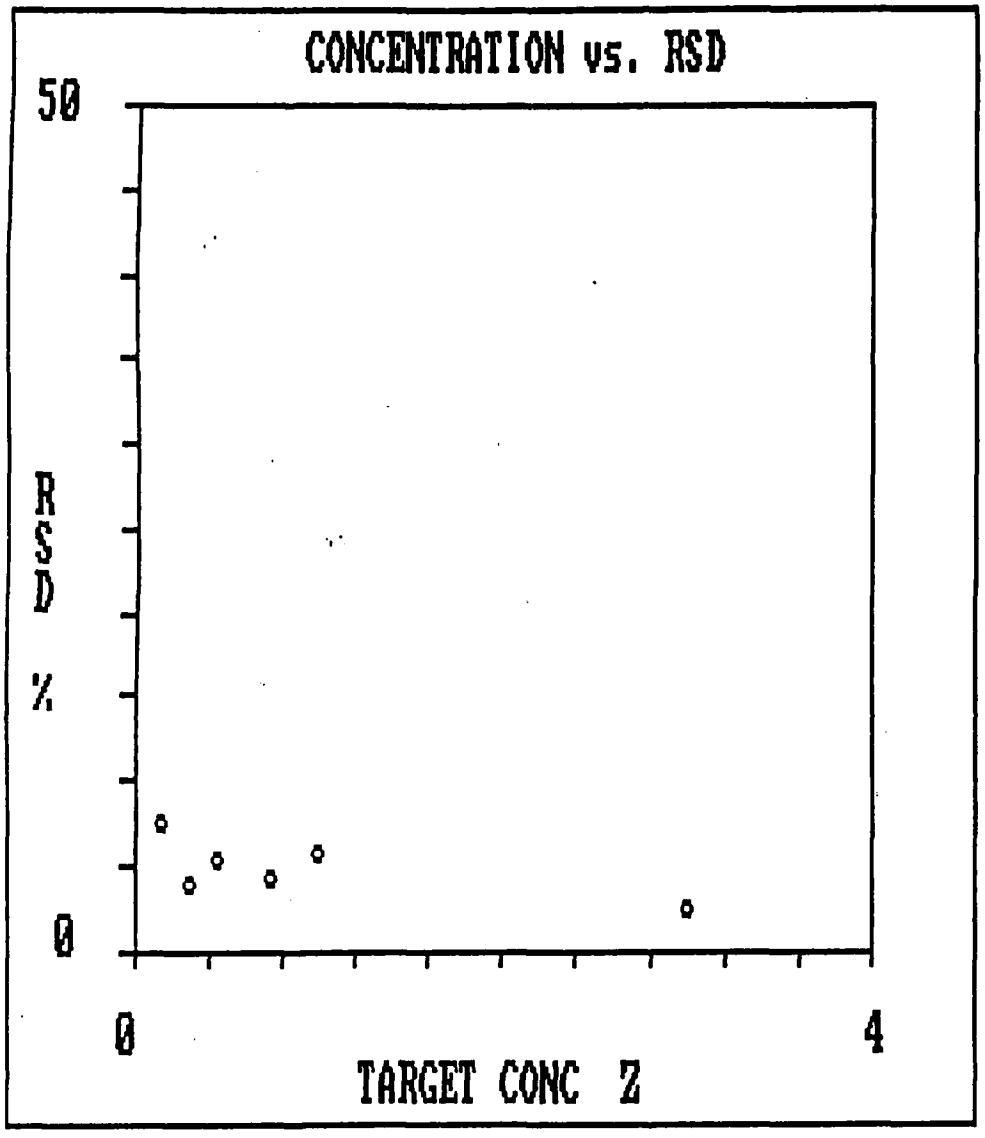
VARIANCE 4 = .1284629

VARIANCE 5 = .1906176

VARIANCE 6 = .6587513

VARIANCE 7 = 1

AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88



RSD % 1 = 0

RSD % 2 = 7.531014

RSD % 3 = 3.947184

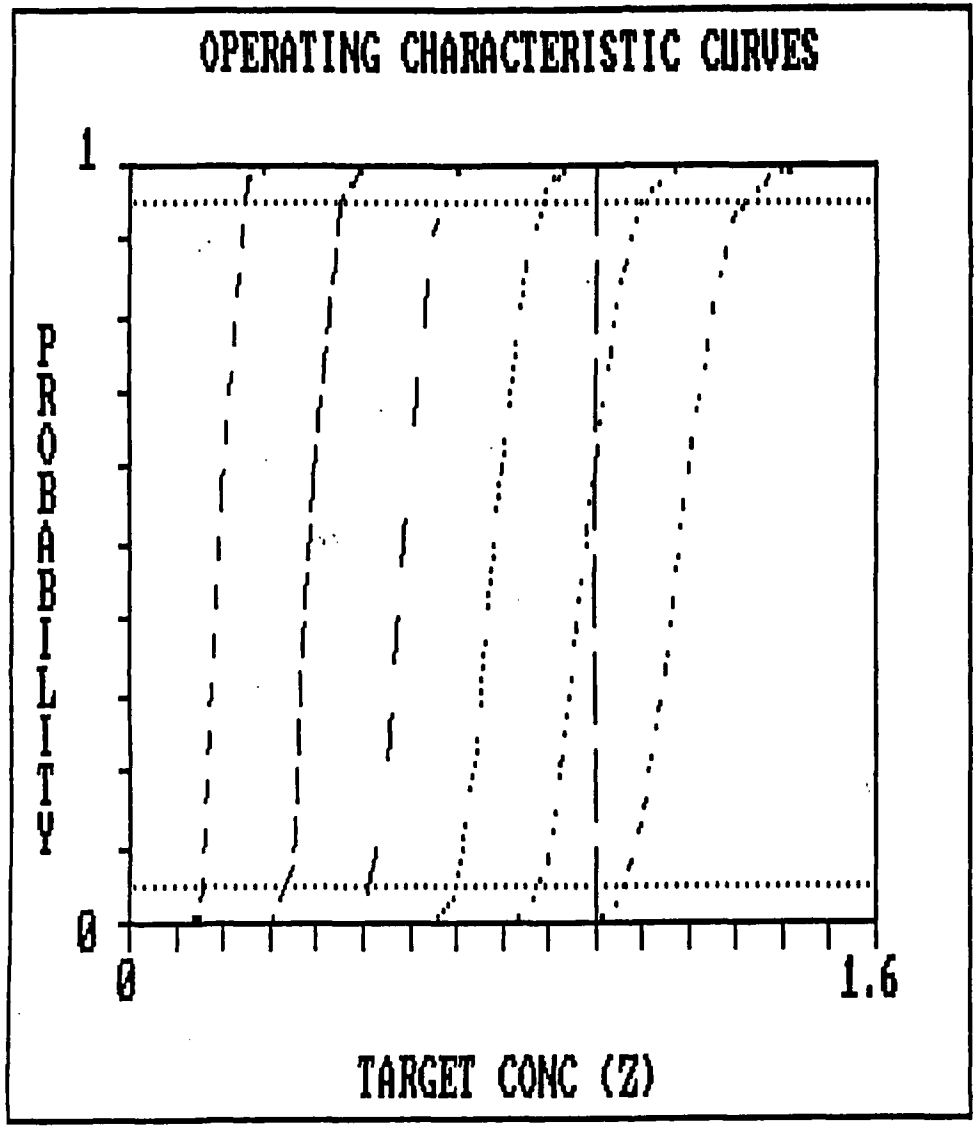
RSD % 4 = 5.100124

RSD % 5 = 4.250239

RSD % 6 = 5.679768

RSD % 7 = 2.340612

AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88



AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88

ALARM SETTINGS

95.0% AT HZD= .908952

97.5% AT HZD= .887861

99.0% AT HZD= .863175

FALSE AT .5Z= 0

FALSE(.05 = .784999

--------- = .2

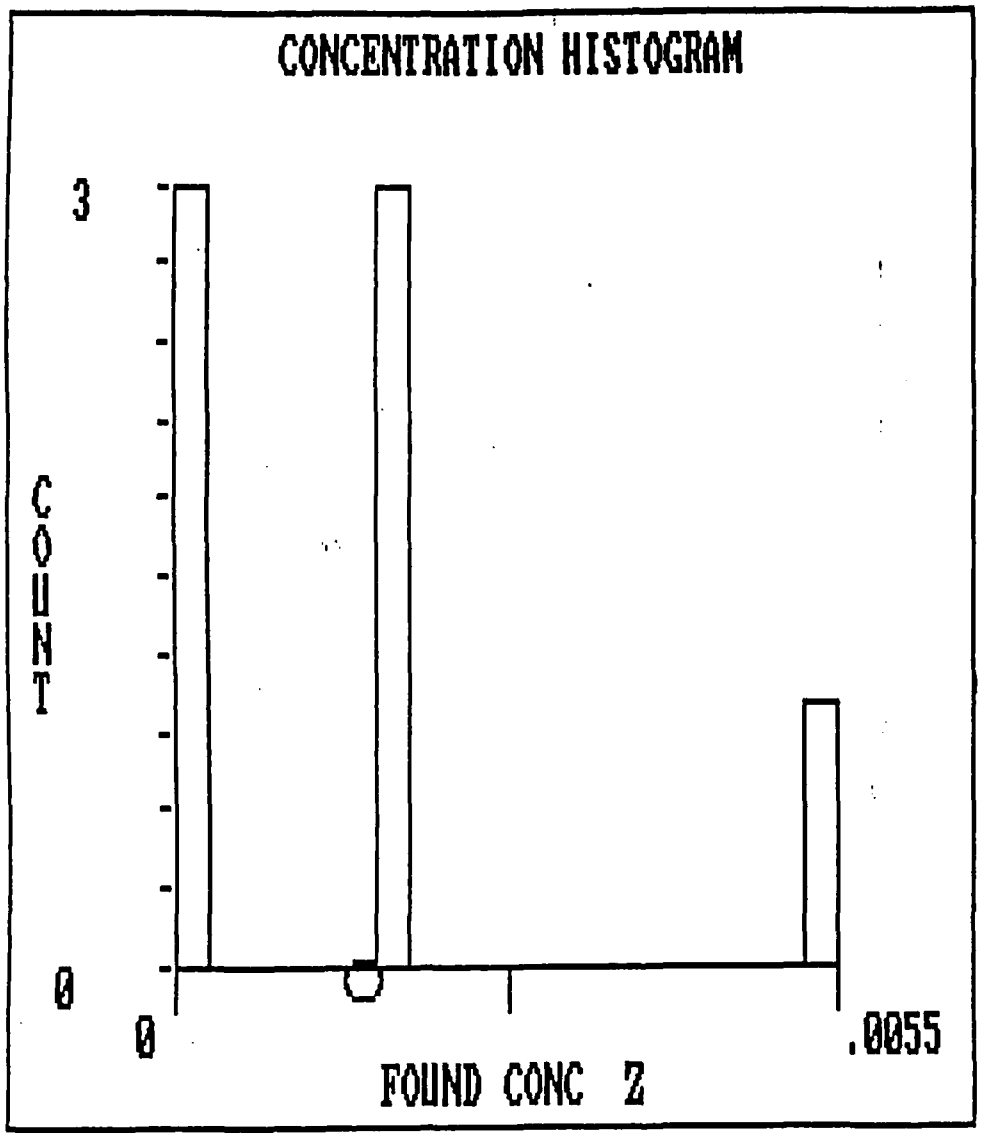
--------- = .4

- - - - - = .6

.... = .8

.... = 1

.... = 1.2



AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88

TARGET CONC.= 0

RANGE = .0055

MEAN (FOUND)= .0015571

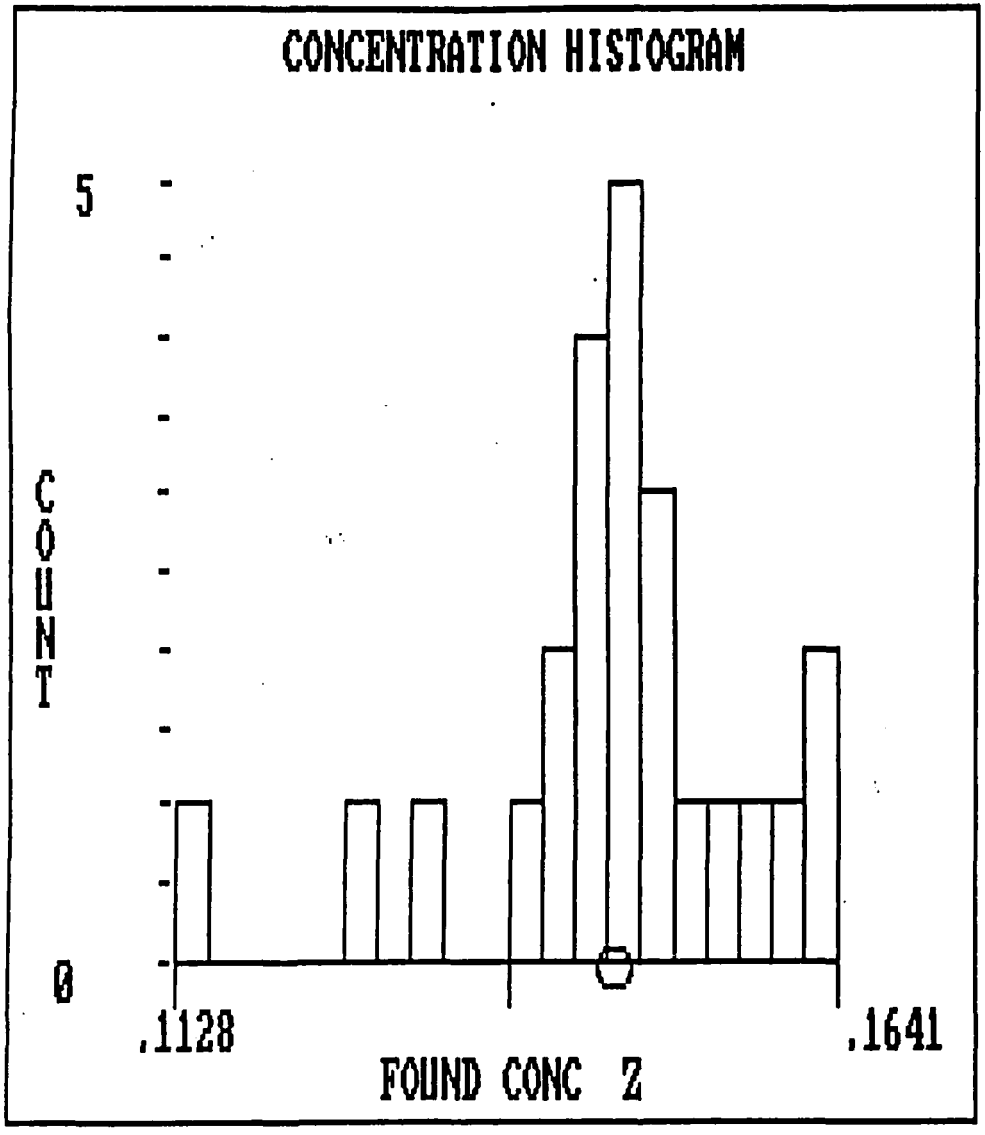
STD DEV = .0019577

TOTAL COUNT = 7

% OF TOTAL = 5.645161

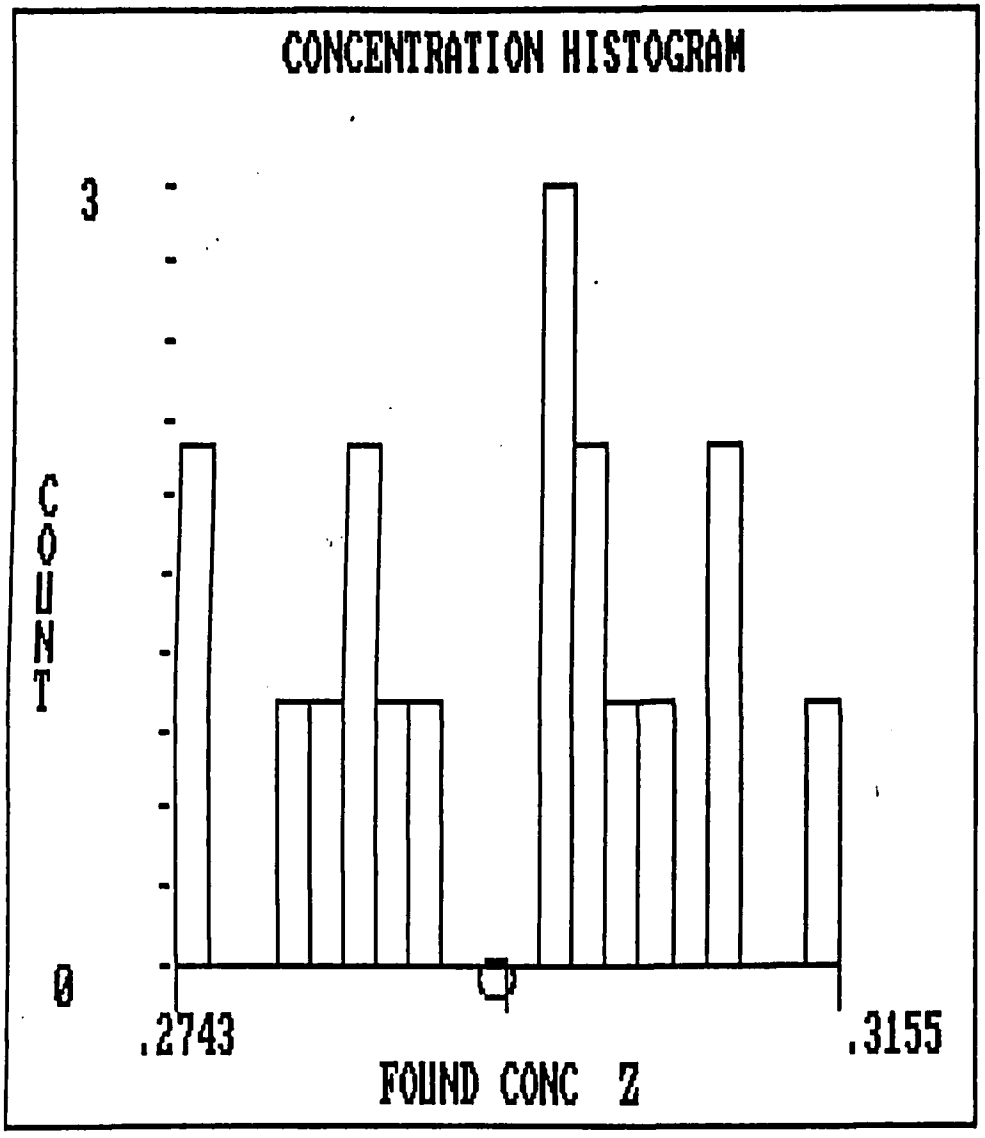
MINIMUM = 0

MAXIMUM = .0055



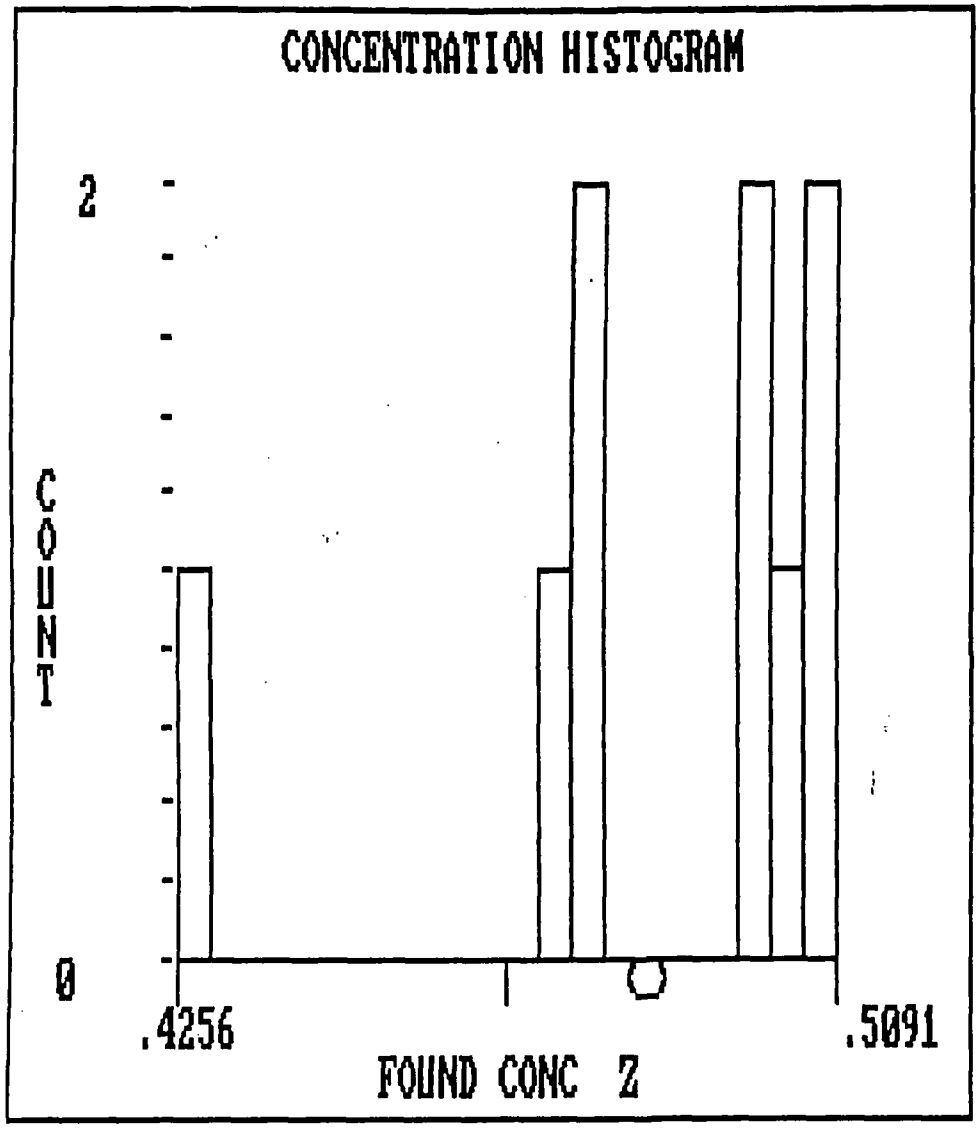
AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88

TARGET CONC.= .1467
RANGE = .0513999
MEAN (FOUND)= .1466291
STD DEV = .01128
TOTAL COUNT = 24
% OF TOTAL = 19.35484
MINIMUM = .1128
MAXIMUM = .1641999



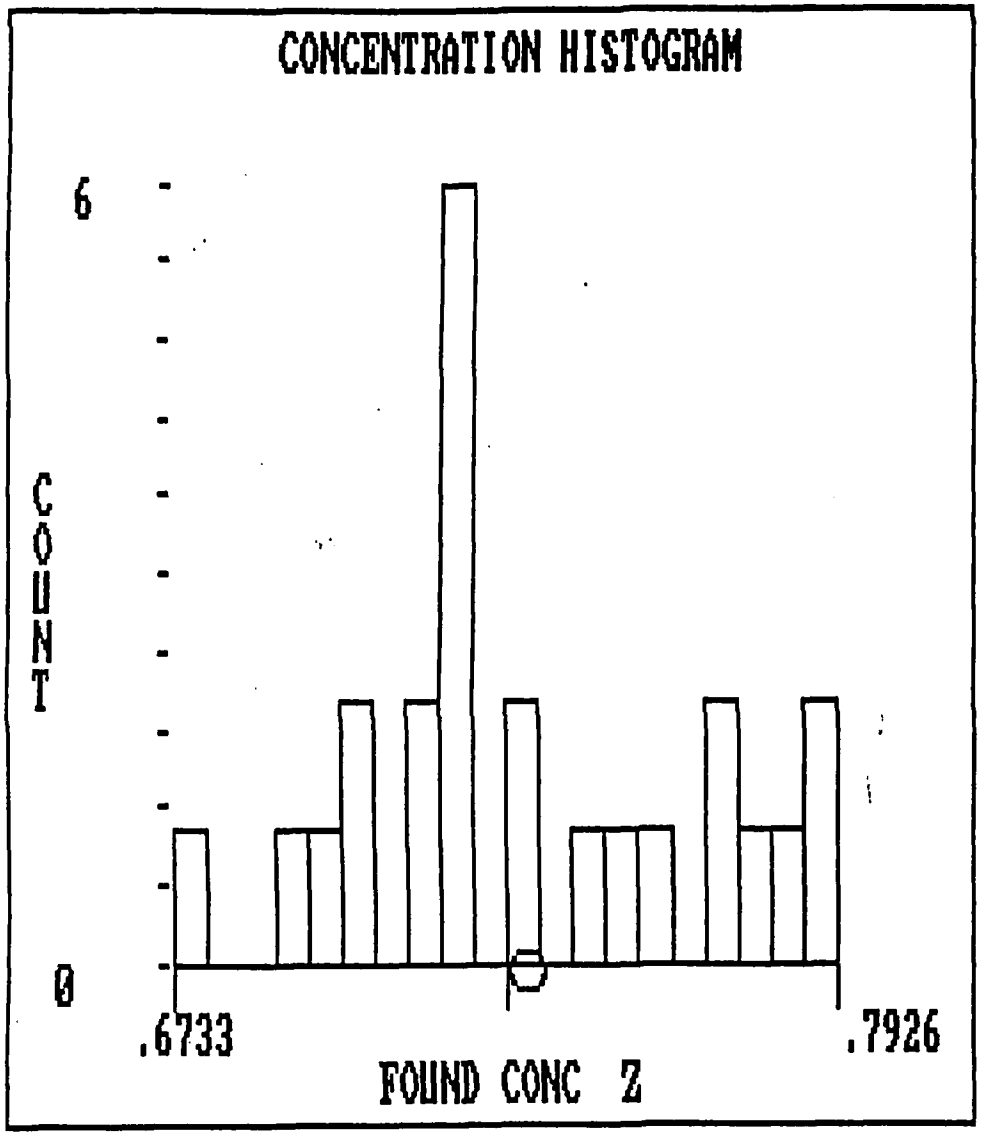
AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88

TARGET CONC.= .2935
RANGE = .0411999
MEAN (FOUND)= .2942944
STD DEV = .0119533
TOTAL COUNT = 18
% OF TOTAL = 14.51613
MINIMUM = .2743
MAXIMUM = .3155



TARGET CONC.= .4403
RANGE = .0835
MEAN (FOUND)= .4851556
STD DEV = .0262442
TOTAL COUNT = 9
% OF TOTAL = 7.258064
MINIMUM = .4256
MAXIMUM = .5091

AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88



AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88

TARGET CONC.= .7339

RANGE = .1192999

MEAN (FOUND)= .7363375

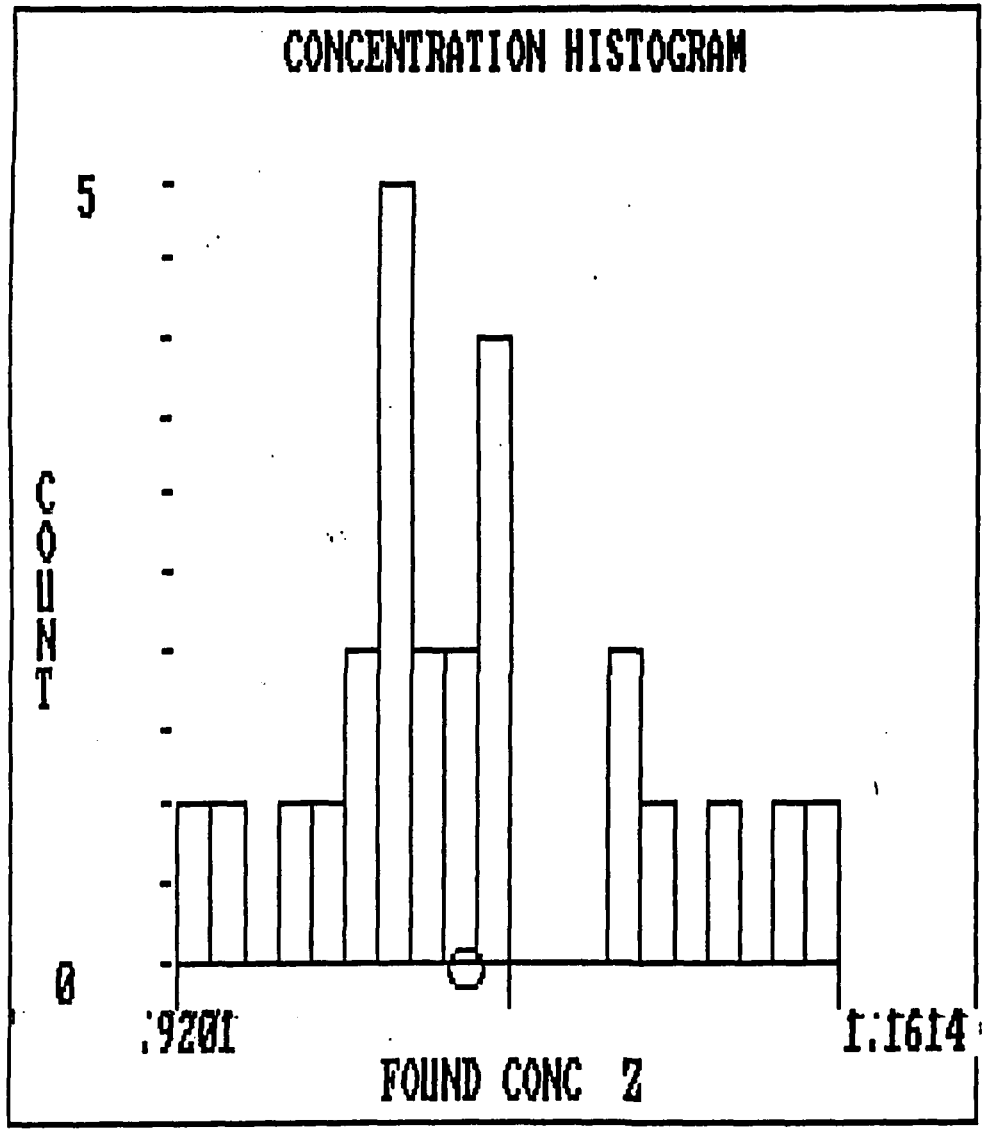
STD DEV = .0319688

TOTAL COUNT = 24

% OF TOTAL = 19.35484

MINIMUM = .6733

MAXIMUM = .7926



TARGET CONC.= 1

RANGE = .2412999

MEAN (FOUND)= 1.025232

STD DEV = .05943

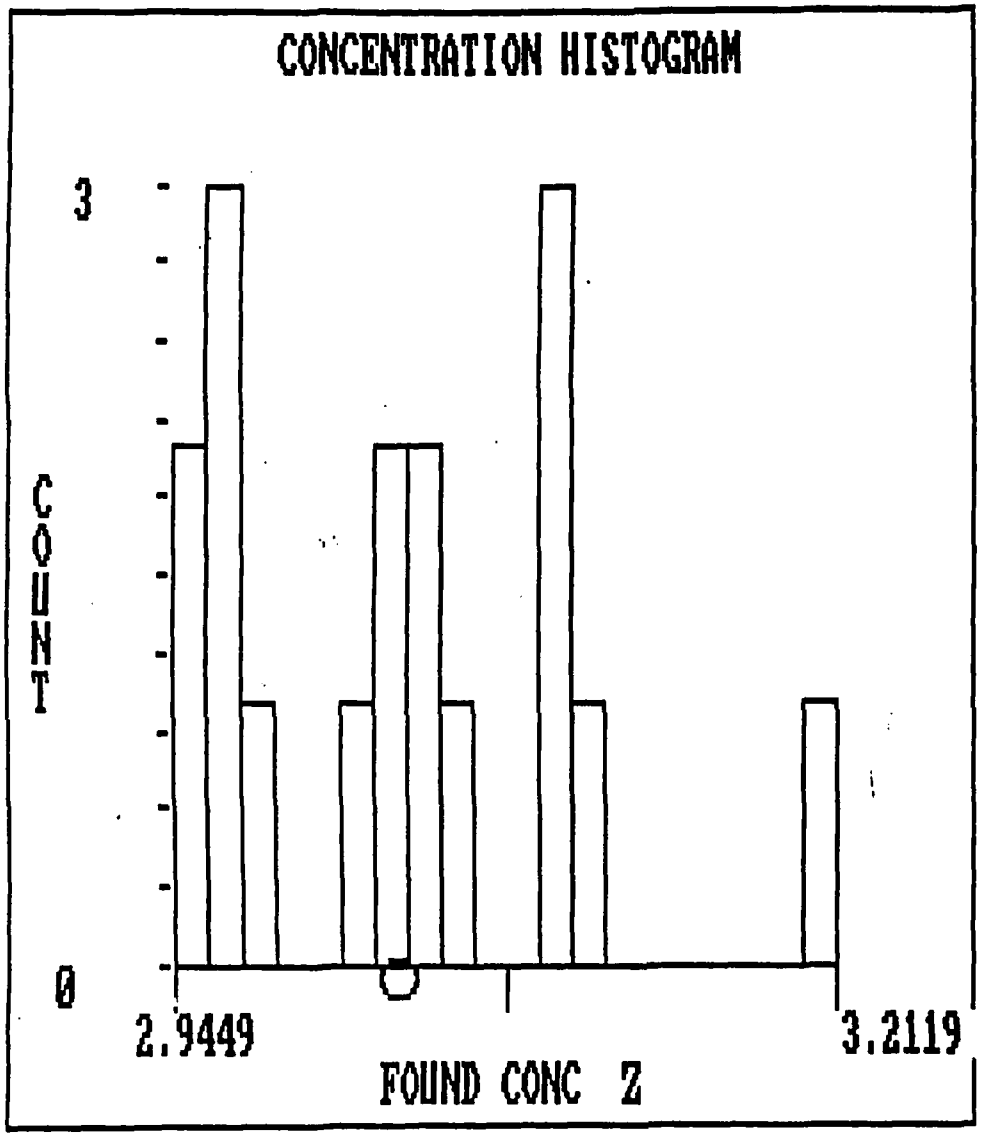
TOTAL COUNT = 25

% OF TOTAL = 20.16129

MINIMUM = .9201

MAXIMUM = 1.1614

AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88



AGENT: GB LAB: CAMDS/EAI DATES: 12-15 JAN 88

TARGET CONC.= 2.9999
RANGE = .2669999
MEAN (FOUND)= 3.0347
STD DEV = .0732226
TOTAL COUNT = 17
% OF TOTAL = 13.70968
MINIMUM = 2.9449
MAXIMUM = 3.2119

TABLE OF DATA

GROUP#	WEIGHT	TARGET	FOUND	YHAT	RESID	Wtd RESID
1.00	6516.54	0.0000	0.0000	0.0006	-0.001	-0.045
1.00	6516.54	0.0000	0.0000	0.0006	-0.001	-0.045
1.00	6516.54	0.0000	0.0000	0.0006	-0.001	-0.045
1.00	6516.54	0.0000	0.0018	0.0006	0.001	0.100
1.00	6516.54	0.0000	0.0055	0.0006	0.005	0.399
1.00	6516.54	0.0000	0.0018	0.0006	0.001	0.100
1.00	6516.54	0.0000	0.0018	0.0006	0.001	0.100
2.00	4022.34	0.1467	0.1513	0.1497	0.002	0.101
2.00	4022.34	0.1467	0.1568	0.1497	0.007	0.449
2.00	4022.34	0.1467	0.1642	0.1497	0.014	0.919
2.00	4022.34	0.1467	0.1467	0.1497	-0.003	-0.191
2.00	4022.34	0.1467	0.1486	0.1497	-0.001	-0.071
2.00	4022.34	0.1467	0.1504	0.1497	0.001	0.044
2.00	4022.34	0.1467	0.1440	0.1497	-0.006	-0.362
2.00	4022.34	0.1467	0.1440	0.1497	-0.006	-0.362
2.00	4022.34	0.1467	0.1614	0.1497	0.012	0.741
2.00	4022.34	0.1467	0.1275	0.1497	-0.022	-1.409
2.00	4022.34	0.1467	0.1394	0.1497	-0.010	-0.654
2.00	4022.34	0.1467	0.1422	0.1497	-0.008	-0.477
2.00	4022.34	0.1467	0.1431	0.1497	-0.007	-0.419
2.00	4022.34	0.1467	0.1486	0.1497	-0.001	-0.071
2.00	4022.34	0.1467	0.1642	0.1497	0.014	0.919
2.00	4022.34	0.1467	0.1467	0.1497	-0.003	-0.191
2.00	4022.34	0.1467	0.1477	0.1497	-0.002	-0.128
2.00	4022.34	0.1467	0.1550	0.1497	0.005	0.335
2.00	4022.34	0.1467	0.1321	0.1497	-0.018	-1.117
2.00	4022.34	0.1467	0.1458	0.1497	-0.004	-0.248
2.00	4022.34	0.1467	0.1522	0.1497	0.002	0.158
2.00	4022.34	0.1467	0.1128	0.1497	-0.037	-2.341
2.00	4022.34	0.1467	0.1440	0.1497	-0.006	-0.362
2.00	4022.34	0.1467	0.1504	0.1497	0.001	0.044
3.00	2727.02	0.2935	0.2990	0.2990	0.000	0.002
3.00	2727.02	0.2935	0.3045	0.2990	0.006	0.289
3.00	2727.02	0.2935	0.3082	0.2990	0.009	0.482
3.00	2727.02	0.2935	0.2743	0.2990	-0.025	-1.288
3.00	2727.02	0.2935	0.2807	0.2990	-0.018	-0.954
3.00	2727.02	0.2935	0.2899	0.2990	-0.009	-0.474
3.00	2727.02	0.2935	0.2862	0.2990	-0.013	-0.667
3.00	2727.02	0.2935	0.2871	0.2990	-0.012	-0.620
3.00	2727.02	0.2935	0.3009	0.2990	0.002	0.101
3.00	2727.02	0.2935	0.2853	0.2990	-0.014	-0.714
3.00	2727.02	0.2935	0.3027	0.2990	0.004	0.195
3.00	2727.02	0.2935	0.3082	0.2990	0.009	0.482
3.00	2727.02	0.2935	0.2834	0.2990	-0.016	-0.813
3.00	2727.02	0.2935	0.2972	0.2990	-0.002	-0.092
3.00	2727.02	0.2935	0.3155	0.2990	0.017	0.863
3.00	2727.02	0.2935	0.2752	0.2990	-0.024	-1.241
3.00	2727.02	0.2935	0.2981	0.2990	-0.001	-0.045
3.00	2727.02	0.2935	0.3009	0.2990	0.002	0.101
4.00	1969.81	0.4403	0.4256	0.4482	-0.023	-1.004

GROUP#	WEIGHT	TARGET	FOUND	YHAT	RESID	Wtd RESID
4.00	1969.81	0.4403	0.4981	0.4482	0.050	2.214
4.00	1969.81	0.4403	0.5027	0.4482	0.054	2.418
4.00	1969.81	0.4403	0.5064	0.4482	0.058	2.582
4.00	1969.81	0.4403	0.4724	0.4482	0.024	1.073
4.00	1969.81	0.4403	0.4770	0.4482	0.029	1.277
4.00	1969.81	0.4403	0.4770	0.4482	0.029	1.277
4.00	1969.81	0.4403	0.4981	0.4482	0.050	2.214
4.00	1969.81	0.4403	0.5091	0.4482	0.061	2.702
5.00	1165.20	0.7339	0.7697	0.7467	0.023	0.784
5.00	1165.20	0.7339	0.7752	0.7467	0.028	0.972
5.00	1165.20	0.7339	0.7926	0.7467	0.046	1.566
5.00	1165.20	0.7339	0.7357	0.7467	-0.011	-0.377
5.00	1165.20	0.7339	0.7587	0.7467	0.012	0.409
5.00	1165.20	0.7339	0.7733	0.7467	0.027	0.907
5.00	1165.20	0.7339	0.6733	0.7467	-0.073	-2.507
5.00	1165.20	0.7339	0.7266	0.7467	-0.020	-0.687
5.00	1165.20	0.7339	0.7266	0.7467	-0.020	-0.687
5.00	1165.20	0.7339	0.7082	0.7467	-0.039	-1.315
5.00	1165.20	0.7339	0.7238	0.7467	-0.023	-0.783
5.00	1165.20	0.7339	0.7330	0.7467	-0.014	-0.469
5.00	1165.20	0.7339	0.7513	0.7467	0.005	0.156
5.00	1165.20	0.7339	0.7834	0.7467	0.037	1.252
5.00	1165.20	0.7339	0.7871	0.7467	0.040	1.378
5.00	1165.20	0.7339	0.6926	0.7467	-0.054	-1.848
5.00	1165.20	0.7339	0.7174	0.7467	-0.029	-1.001
5.00	1165.20	0.7339	0.7238	0.7467	-0.023	-0.783
5.00	1165.20	0.7339	0.7036	0.7467	-0.043	-1.472
5.00	1165.20	0.7339	0.7155	0.7467	-0.031	-1.066
5.00	1165.20	0.7339	0.7256	0.7467	-0.021	-0.721
5.00	1165.20	0.7339	0.6990	0.7467	-0.048	-1.629
5.00	1165.20	0.7339	0.7266	0.7467	-0.020	-0.687
5.00	1165.20	0.7339	0.7495	0.7467	0.003	0.094
6.00	796.82	1.0000	1.1137	1.0173	0.096	2.722
6.00	796.82	1.0000	1.1440	1.0173	0.127	3.577
6.00	796.82	1.0000	1.1614	1.0173	0.144	4.068
6.00	796.82	1.0000	0.9201	1.0173	-0.097	-2.743
6.00	796.82	1.0000	0.9908	1.0173	-0.026	-0.748
6.00	796.82	1.0000	1.0128	1.0173	-0.004	-0.127
6.00	796.82	1.0000	0.9394	1.0173	-0.078	-2.198
6.00	796.82	1.0000	0.9926	1.0173	-0.025	-0.697
6.00	796.82	1.0000	1.0321	1.0173	0.015	0.418
6.00	796.82	1.0000	1.0192	1.0173	0.002	0.054
6.00	796.82	1.0000	1.0357	1.0173	0.018	0.520
6.00	796.82	1.0000	1.0376	1.0173	0.020	0.574
6.00	796.82	1.0000	1.0816	1.0173	0.064	1.816
6.00	796.82	1.0000	1.0844	1.0173	0.067	1.895
6.00	796.82	1.0000	1.0954	1.0173	0.078	2.205
6.00	796.82	1.0000	0.9605	1.0173	-0.057	-1.603
6.00	796.82	1.0000	0.9779	1.0173	-0.039	-1.112
6.00	796.82	1.0000	0.9935	1.0173	-0.024	-0.671

GROUP#	WEIGHT	TARGET	FOUND	YHAT	RESID	Wtd RESID
6.00	796.82	1.0000	0.9972	1.0173	-0.020	-0.567
6.00	796.82	1.0000	0.9880	1.0173	-0.029	-0.827
6.00	796.82	1.0000	1.0091	1.0173	-0.008	-0.231
6.00	796.82	1.0000	1.0311	1.0173	0.014	0.390
6.00	796.82	1.0000	0.9972	1.0173	-0.020	-0.567
6.00	796.82	1.0000	0.9972	1.0173	-0.020	-0.567
6.00	796.82	1.0000	1.0183	1.0173	0.001	0.029
7.00	150.55	2.9999	3.1027	3.0506	0.052	0.639
7.00	150.55	2.9999	3.1091	3.0506	0.058	0.717
7.00	150.55	2.9999	3.2119	3.0506	0.161	1.979
7.00	150.55	2.9999	2.9495	3.0506	-0.101	-1.241
7.00	150.55	2.9999	2.9623	3.0506	-0.088	-1.084
7.00	150.55	2.9999	3.0954	3.0506	0.045	0.549
7.00	150.55	2.9999	2.9449	3.0506	-0.106	-1.297
7.00	150.55	2.9999	3.0256	3.0506	-0.025	-0.307
7.00	150.55	2.9999	3.0440	3.0506	-0.007	-0.081
7.00	150.55	2.9999	2.9587	3.0506	-0.092	-1.128
7.00	150.55	2.9999	2.9605	3.0506	-0.090	-1.106
7.00	150.55	2.9999	2.9788	3.0506	-0.072	-0.881
7.00	150.55	2.9999	3.0302	3.0506	-0.020	-0.251
7.00	150.55	2.9999	3.0605	3.0506	0.010	0.121
7.00	150.55	2.9999	3.0128	3.0506	-0.038	-0.464
7.00	150.55	2.9999	3.0440	3.0506	-0.007	-0.081
7.00	150.55	2.9999	3.0990	3.0506	0.048	0.594

APPENDIX B

Weighted Regression Technique

The regression line for the experimental data is determine using a weighting procedure as described by Draper and Smith[1] and further described in terms of analytical procedures and confidence limits by Garden, et. al.[2]. The program code is a modification of the method used by Southern Research Institute in its statistical analysis of experimental dat for the PM Cml Demil[3]. The weighting procedure in CERTIFY is used to obtain the best fit linear regression line and to calculate the confidence limits about that regression line.

The weighting is done assuming a linear function of standard deviation with target concentration. The independent variable is the target concentration and the dependent variable, the found concentration. Standard deviations at each target concentration are calculated and a first order polynomial is fitted to determine standard deviation given target concentration. This shown in Equation 1.

$$s(y_g) = a_g + b_g x_g \qquad (1)$$

where subscript g denotes group

Once this regression is determined, the weight for a given target concentration can be determined from Equation 2.

$$w_i = (a_g + b_g x_i)^{-2} \qquad (2)$$

And finally, the weighted regression coefficients are determined using Equations 3 and 4 to fit Found Concentration versus Target Concentration according to Equation 5.

$$b_o = \frac{\sum w_i y_i \sum w_i x_i^2 - \sum w_i x_i \sum w_i y_i}{\sum w_i \sum w_i x_i^2 - \left(\sum w_i x_i\right)^2} \qquad (3)$$

$$b_1 = \frac{\sum w_i \sum w_i x_i y_i - \sum w_i x_i \sum w_i y_i}{\sum w_i \sum w_i x_i^2 - \left(\sum w_i x_i\right)^2} \qquad (4)$$

$$y = b_o + b_1 x \qquad (5)$$

Once a regression line is determined and the standard deviation can be calculated for each target concentration, confidence bounds are determined at the 95% confidence limits for a future observation of Found Concentration according to the method described in AMCP 706-110[4] with the appropriate weighting modified to include the effects of the weighting function. Additionally, a 5% relative error is added to account for deviations in flowrate.

A mention of the method of determination of the Students t statistic is made here. The integral of Equation 7 is solved assuming a negative infinity of -8 and a 15 point Gaussian Quadrature. This method allows calculation of the t statistic to a least 3 decimal places. The appropriate value of probability is converged on using successive substitution to an error of +/- 0.005. This method of calculating this statistic is also used in construction of the OC Curve to be described in Appendix C.

[1] Applied Regression Analysis, N.R. Draper and H. Smith, 2nd Ed., (John Wiley and Sons, New York, 1981), pp. 108-116.

[2] Garden, J.S., Mitchell, D.G., and W.N. Mills, "Nonconstant Variance Regression Techniques for Calibration-Curve-Based Analysis", Anal. Chem., 1980, pp. 2310-2315.

[3] Summary of the Weighted Hubaux-Vos Analysis Procedure used at Southern Research Institute, letter to Mr. Michael Gooden/AMCPEO-CDM, DRAFT discussion, 5 Feb 88.

[4] Engineering Design Handbook, Experimental Statistics, Section 1, AMCP 706-110, Headquarters, U.S. Army Materiel Command, Dec 69.

APPENDIX C

Calculations of the OC Curves

The OC (operating characteristics) curves are calculated using the calculated standard deviation at the hazard level. The calculation is made using the regression of standard deviation with target concentration. Essentially, the probability of alarm is determined from successive substitution of values for the t statistic using convergence tolerances of +/- 0.005. The confidence limits used in generation of the plots and tables for given alarm settings are 97.5% limits based on a one sided t statistic. The methodology for calculation of the t statistic itself was described in Appendix B.

APPENDIX D

Outlier Testing

Outlier testing is done based on methods suggested in the ASTM manual for outlier testing[1]. The method is based on calculation of the skewness and kurtosis of the data set in questing and comparison to tabulated statistics given by Barnett and Lewis[2]. The method consists of calculating the skewness according to Equation 1 and the kurtosis according to Equation 2.

$$\text{skewness} = \frac{\sqrt{n}\sum (y_i - \bar{y})^3}{\left[\sum (y_i - \bar{y})^2\right]^{3/2}} \qquad (1)$$

$$\text{kurtosis} = \frac{n\sum (y_i - \bar{y})^4}{\left[\sum (y_i - \bar{y})^2\right]^2} - 2 \qquad (2)$$

Each of these is compared to the tabulated maximum allowable values at the 1% level. Exceeding these values for the given number of target concentrations (intermediate values being determined by linear interpolation and target concentrations in excess of 1000 assuming the value at 1000) causes the data point farthest from the mean to be discarded and the determination repeated on the data set minus the determined outlier. Bounds on the number of outliers allowed are set at:

$$\text{maximum number of outliers} = (n)^{1/2}$$

$$\text{minimum number of data points} = 5$$

In addition to determining outlying data points, these tests say something about the normality of the data set.

[1] Standard Practice for Dealing with Outlying Observations, ANSI/ASTM E 178-80, Jun 80, pp. A-7.

[2] Outliers in Statistical Data, V. Barnett and T. Lewis, (John Wiley and Sons, New York, 1978), pp. 312.